

#### LA-UR-21-22043

Approved for public release; distribution is unlimited.

Title: Impact of nuclear data validation with uncertainty quantification and

diverse benchmarks on criticality safety

Author(s): Clark, Alexander Rich

Intended for: Interview for Scientist 2 position in XCP-7: Radiation Transport

**Applications** 

Issued: 2021-03-01





#### Impact of nuclear data validation with uncertainty quantification and diverse benchmarks on criticality safety

Alexander R. Clark, Ph.D., E.I.

XCP-5: Materials and Physical Data

March 3rd, 2021

Interview for Scientist 2 position in XCP-7: Radiation Transport Applications

LA-UR-21-xxxxx



#### **Outline**

#### **Dissertation research**

- Introduction and motivation
- Model calibration process
- Model calibration applied to neutron multiplicity counting (NMC) measurements
- Summary and conclusions

#### Postdoctoral research

- Introduction and motivation
- Pulsed-sphere measurements
- SA applied to pulsed-sphere TOF spectra
- Summary and future work

#### **Benefits to criticality safety**

- Nuclear data adjustment accounting for random and systematic uncertainties resulted in improved neutron multiplicity counting simulations
- Combination of critical benchmarks and pulsed sphere measurements in nuclear data validation can provide tighter constraint on fission parameters



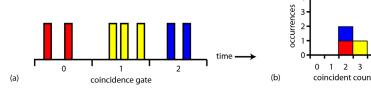
#### Using neutron multiplicity counting to adjust cross sections

- Cross section evaluation via critical experiments and reaction rate measurements has led to their over-calibration for some applications
- ENDF/B-VII.1 cross sections (Pu-239  $\overline{\nu}$ ) do not adequately predict subcritical experiments
- Neutron multiplicity counting (NMC) is a method of non-destructive analysis of SNM assemblies
  - Each NMC distribution moment is a function of the cross sections raised to the power of the moment's order
  - Higher-order NMC distribution moments are more sensitive to the cross sections than the mean (first moment)
  - Model calibration applied to higher-order NMC distribution moments produced more accurately simulated NMC experiments with reduced uncertainty

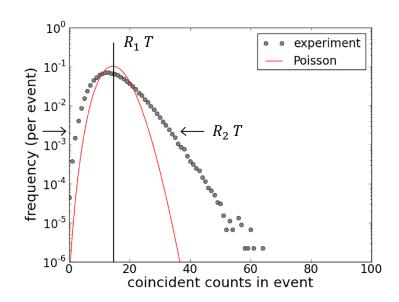


# Characteristics of neutron multiplicity counting

- Neutron multiplicity counting (NMC) accumulates distribution of coincident neutron counts
- Independent neutron emissions characterized by Poisson distribution
- Fission-chain reactions are described by generalized Poisson distribution
- Excess variance in NMC distribution is characteristic of multiplying material
- Need higher-order NMC distribution moments to characterize SNM assemblies



Accumulation of NMC distribution

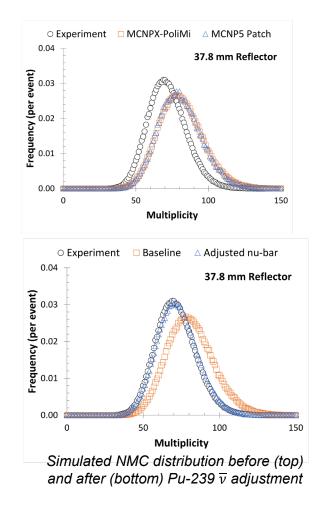


NMC and Poisson distributions with the same mean



# Adjusting the Pu-239 $\overline{\nu}$ to better predict counting distribution

- Simulations of NMC of a 4.5-kg sphere of weapons-grade plutonium metal (BeRP ball) overpredicted NMC distribution moments
- Small reduction in Pu-239  $\overline{\nu}$  improved accuracy of simulated moments
- ENDF/B-VII.1 Pu-239  $\overline{\nu}$  adjusted to match JEZEBEL critical experiments





#### Model calibration overview

#### Sensitivity Uncertainty Parameter Analysis (SA) Quantification Estimation (PE) (UQ) Adjoint- Model First-order based first calibration propagation derivatives of Best-estimate Sensitivity uncertainty cross of detector sections and Detector response to covariances response cross covariance sections



#### Sensitivity Analysis (SA)

- Adjointbased first derivatives
- Sensitivity of detector response to cross sections

# Quantification (UQ)

- First-order propagation of uncertainty
- Detector response covariance

- Model calibration
- Best-estimate cross sections and covariances



## Description of the forward transport equation

 Describes a balance of production and loss terms for expected number of neutrons:

$$L\psi = \widetilde{Q} = \overline{\nu}_{Sf}S$$

$$L = \underbrace{\widehat{\Omega} \cdot \overline{V}}_{\text{streaming loss}} + \underbrace{\widehat{\Sigma}_t}_{\text{interaction loss}} - \underbrace{\int_{4\pi} d\Omega' \int_{0}^{\infty} dE' \Sigma_s}_{\text{scatter source}} - \underbrace{\frac{\chi}{4\pi} \int_{4\pi} d\Omega' \int_{0}^{\infty} dE' \overline{\nu} \Sigma_f}_{\text{scatter source}}$$

*L*: Forward transport operator

 $\psi$ : Forward angular flux

S: Spontaneous fission source rate density and spectrum

 $\Sigma_t$ ,  $\Sigma_s$ ,  $\overline{\nu}\Sigma_f$ : Macroscopic total, scatter, and fission neutron production cross sections  $\chi$ : Fission neutron energy spectrum

## Description of the adjoint transport equation

Counterpart to the forward NTE:

$$L^*\psi_1^* = Q_1^*$$
 
$$L^* = -\widehat{\Omega} \cdot \nabla + \Sigma_t - \int_{4\pi} d\Omega' \int_0^\infty dE' \Sigma_s - \overline{\nu} \Sigma_f \int_{4\pi} d\Omega' \int_0^\infty dE' \frac{\chi}{4\pi}$$

- L\*: adjoint transport operator
- $\psi_1^*$ : Adjoint flux, "importance" of source neutrons to the mean count rate

# Second-moment adjoint transport equation

$$L^*\psi_2^* = Q_2^*$$
 
$$Q_2^* = \overline{\nu(\nu - 1)}\Sigma_f I_1^2$$
 
$$I_1 = \int d\Omega' \int dE' \frac{\chi}{4\pi} \psi_1^*$$

- Obtained from Muñoz-Cobo stochastic transport equation
- *L*\* is the usual adjoint transport operator
- $Q_2^*$  is defined in terms of  $\psi_1^*$
- $\psi_2^*$  is calculable using a standard transport solver



## Form of the detector response moments

• First-moment detector response (mean count rate):

$$R_1 = \langle \psi, Q_1^* \rangle = \langle \psi, \sigma_d \rangle$$

 Equations for higher-order adjoint fluxes have the same form as usual adjoint NTE with special fixed-source terms:

$$L^*\psi_q^* = Q_q^*, q = 1,2,...$$

• Higher-order detector responses are computed like  $R_1$ :

$$R_q = \langle \psi, Q_q^* \rangle + \langle S, Q_{q,Sf}^* \rangle$$



## **Second-moment detector response**

$$\begin{split} R_2 &= \langle \psi, Q_2^* \rangle + \left\langle S, Q_{2,sf}^* \right\rangle \\ Q_2^* &= \overline{\nu(\nu - 1)} \Sigma_f I_1^2, \, Q_{2,sf}^* = \overline{\nu(\nu - 1)}_{sf} I_{1,sf}^2 \\ I_1 &= \int d\Omega' \int dE' \frac{\chi}{4\pi} \psi_1^*, I_{1,sf} = \int d\Omega' \int dE' \frac{\chi_{sf}}{4\pi} \psi_1^* \end{split}$$

- $\psi_1^*$  is a function of the cross sections to the first power
- $Q_2^*$  is proportional to the square of the cross sections



## Benefit of adjoint-based sensitivity analysis

 Adjoint-based approach allows the sensitivity to be computed with few transport solves

$$\frac{\partial R_1}{\partial \alpha} = \left\langle \frac{\partial Q_1^*}{\partial \alpha}, \psi \right\rangle + \left\langle \psi_1^*, \frac{\partial Q}{\partial \alpha} - \frac{\partial L}{\partial \alpha} \psi \right\rangle$$

- Derivative of flux is computationally expensive because it implicitly depends on the cross sections
- Sensitivity of higher-order detector response moments have a similar form

- Adjointbased first derivatives
- Sensitivity of detector response to cross sections

#### Uncertainty Quantification (UQ)

- First-order propagation of uncertainty
- Detector response covariance

- Model calibration
- Best-estimate cross sections and covariances



## Uncertainty quantification for measured responses

- Contribution from random source of uncertainty
  - · Relative response uncertainty reduced by longer counting
- Contribution from systematic source of uncertainty
  - Cannot physically vary most measurement parameters
  - Instead quantify sensitivities via varying measurement parameters in high-fidelity simulations
  - Response uncertainty reduced by knowing the measurement parameters more precisely

$$[\operatorname{cov}(\boldsymbol{R}_m, \boldsymbol{R}_m)]_{\boldsymbol{p}} = \left(\frac{\partial \boldsymbol{R}_m}{\partial \boldsymbol{p}}\Big|_{\boldsymbol{p}=\boldsymbol{p}^0}\right)^T \operatorname{cov}(\boldsymbol{p}, \boldsymbol{p}) \left(\frac{\partial \boldsymbol{R}_m}{\partial \boldsymbol{p}}\Big|_{\boldsymbol{p}=\boldsymbol{p}^0}\right)$$

Covariance between measured responses

$$cov(\mathbf{R}_m, \mathbf{R}_m) = [var(\mathbf{R}_m)]_N + [cov(\mathbf{R}_m, \mathbf{R}_m)]_{\mathbf{p}}$$



## Uncertainty quantification for simulated responses

- Contribution from model representation errors
  - · Quantified via varying features of the experiment or the phase-space discretization
  - · Response uncertainty reduced via higher-fidelity simulations
- Contribution from nuclear cross sections
  - Cross section covariances are determined from cross section measurement uncertainty
  - Response uncertainty reduced by knowing cross sections more precisely or through model calibration

$$[\operatorname{relcov}(R,R)]_{\alpha} = S_{R,\alpha}^{\mathrm{T}} \operatorname{relcov}(\alpha,\alpha) S_{R,\alpha}$$

Covariance between simulated responses

$$relcov(R, R) = [relcov(R, R)]_{\alpha}$$



- Adjointbased first derivatives
- Sensitivity of detector response to cross sections

# Quantification (UQ)

- First-order propagation of uncertainty
- Detector response covariance

#### Parameter Estimation (PE)

- Model calibration
- Best-estimate cross sections and covariances



# Model calibration using an extended Kalman filter

- Determine best-estimate cross sections and covariances that give optimum agreement between measured and simulated responses
- Bayesian inference method can use prior information about cross section distribution
- Nominal cross section values and corresponding covariances may be described by a multivariate Gaussian distribution
- Extended Kalman filter (EKF) is a method that produces best-estimate cross sections and covariances by using:
  - Prior cross section distribution
  - Measured NMC distribution moments



# **Extended Kalman filter algorithm**

Prediction step

$$R_q^0 = \langle \psi, Q_q^* \rangle|_{\alpha = \alpha^0} + \langle S, Q_{q,Sf}^* \rangle|_{\alpha = \alpha^0}, \quad \operatorname{cov}(\mathbf{R}^0, \mathbf{R}^0) = \left(\frac{\partial \mathbf{R}^0}{\partial \alpha}|_{\alpha = \alpha^0}\right)^T \operatorname{cov}(\mathbf{\alpha}^0, \mathbf{\alpha}^0) \left(\frac{\partial \mathbf{R}^0}{\partial \alpha}|_{\alpha = \alpha^0}\right)$$

Update step

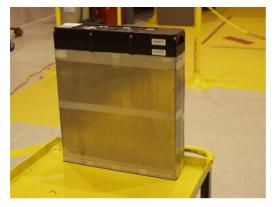
$$K = \frac{\operatorname{cov}(\boldsymbol{\alpha}^{0}, \boldsymbol{\alpha}^{0}) \left( \frac{\partial \boldsymbol{R}^{0}}{\partial \boldsymbol{\alpha}} |_{\boldsymbol{\alpha} = \boldsymbol{\alpha}^{0}} \right)}{\operatorname{cov}(\boldsymbol{R}_{m}, \boldsymbol{R}_{m}) + \operatorname{cov}(\boldsymbol{R}^{0}, \boldsymbol{R}^{0})}$$

$$\alpha^1 = \alpha^0 + K(R_m - R^0), \quad \text{cov}(\alpha^1, \alpha^1) = \left(I - K\left(\frac{\partial R^0}{\partial \alpha}|_{\alpha = \alpha^0}\right)^T\right) \text{cov}(\alpha^0, \alpha^0)$$



#### **Detector response and sensitivity** calculations

- Obtained 44-group cross sections and their covariances from SCALE
- Performed 1D PARTISN simulations of NMC of BeRP ball with nPod
  - Bare and 3.8 cm polyethylene-reflected configurations
  - Simplified composition of plutonium metal (Pu-239, 240) and polyethylene reflector (H-1, C-12)
  - nPod modeled as adjoint source on outer boundary



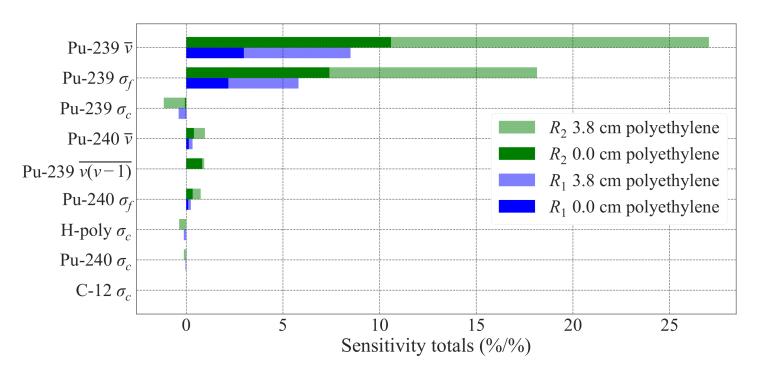
nPod neutron multiplicity counter



BeRP ball nested in polyethylene reflectors

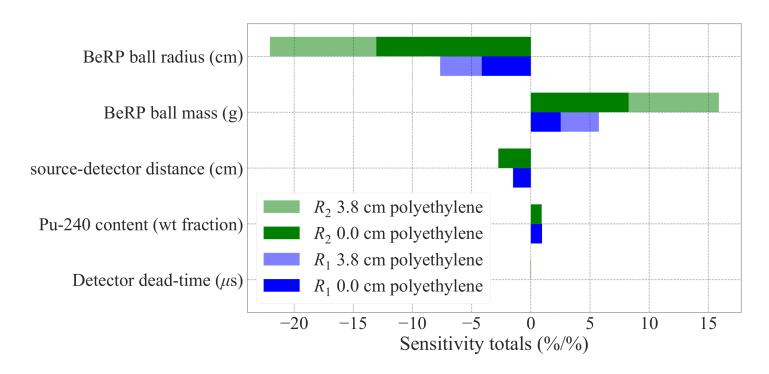


# $R_1$ and $R_2$ relative sensitivity totals



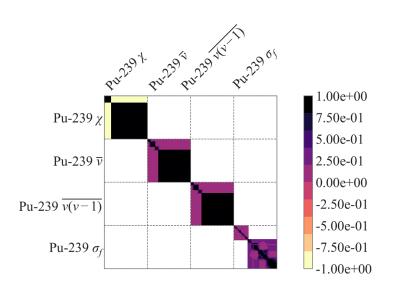


# Sensitivity totals for the measured $R_1$ and $R_2$

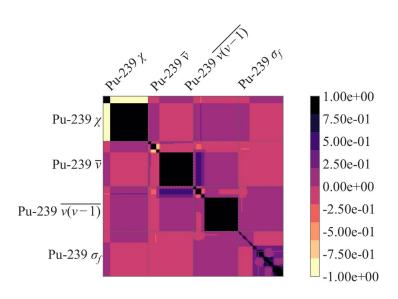




### Nominal and adjusted cross section correlations



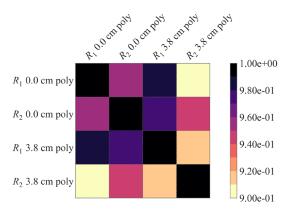
Correlations between the cross sections before the model calibration



Correlations between the cross sections after the model calibration

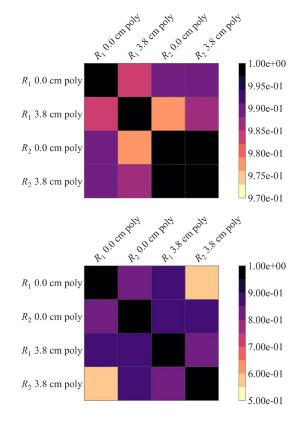


#### Measured and simulated response correlations



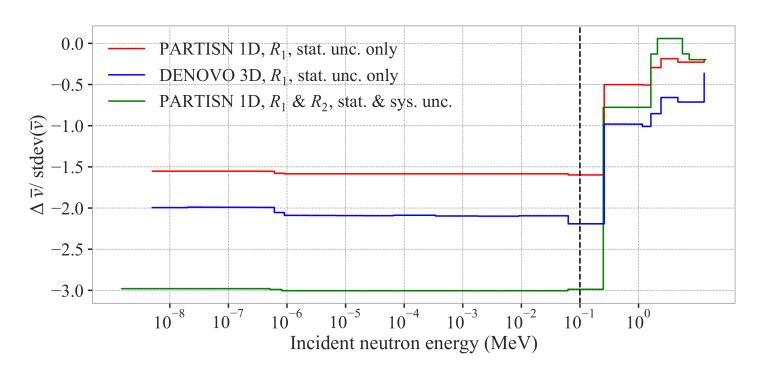
Correlations between the measured responses due to the measurement parameters

Correlations between the nominal (top-right) and adjusted (bottom-right) simulated responses due to the cross sections



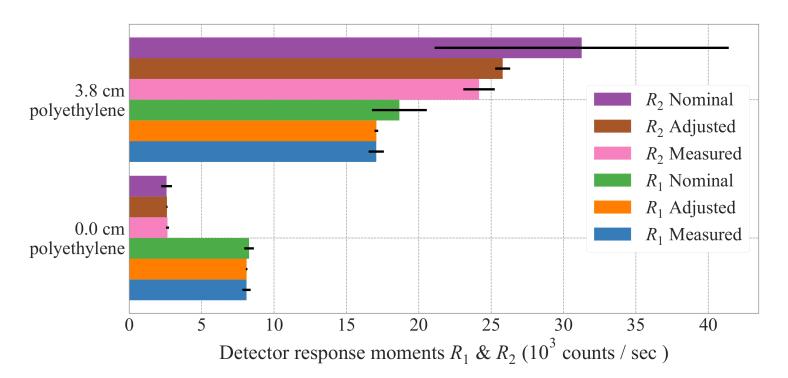


# Optimal adjustment to the Pu-239 $\overline{\nu}$





# $R_1$ and $R_2$ comparison to experiment





# **Summary and conclusions**

- Calculated variance in the second moment detector response due to both random and systematic sources of uncertainty
- Applied an EKF to identify best-estimate cross sections and their covariances
- Demonstrated that NMC experiments were more accurately simulated with reduced uncertainty
- Adjustment to the cross sections is similar in trend to previous work but larger in magnitude due to inclusion of  $R_2$  and systematic uncertainties



#### **Outline**

#### Dissertation research

- Introduction and motivation
- Model calibration process
- Model calibration applied to neutron multiplicity counting (NMC) measurements
- Summary and conclusions

#### Postdoctoral research

- Introduction and motivation
- Pulsed-sphere measurements
- SA applied to pulsed-sphere TOF spectra
- Summary and future work

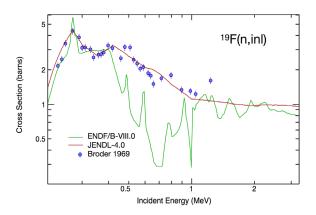
#### **Benefits to criticality safety**

- Nuclear data adjustment accounting for random and systematic uncertainties resulted in improved neutron multiplicity counting simulations
- Combination of critical benchmarks and pulsed sphere measurements in nuclear data validation can provide tighter constraint on fission parameters



# Identification of discrepant nuclear data with machine learning

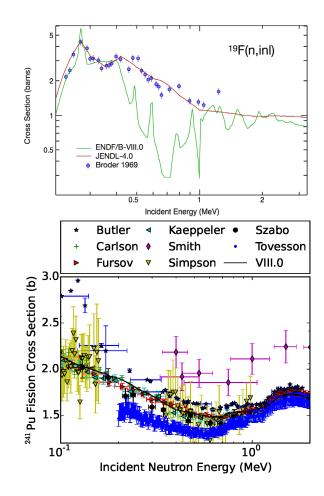
- Deficiencies in nuclear data can have significant impact on many applications, including determining USLs for criticality safety
- Previous Machine Learning project had already identified discrepant nuclear data that most contributed to bias between measured and simulated critical benchmark responses (funded by NCSP-ASC [ATDM-PEM-V&V])
- LDRD-DR project, EUCLID, objective is "to design small-scale experiments that address needs and deficiencies in nuclear data"



- P. Grechanuk, M. E. Rising, and T. S. Palmer, "Using Machine Learning Methods to Predict Bias in Nuclear Criticality Safety," *J. Comput. Theor.* Transp., 47:4-6, 552-565
- D. Neudecker, O. Cabellos, A. R. Clark et al., "Enhancing Nuclear Data Validation Analysis by Using Machine Learning," Submitted Sept. 2019 to Nucl Data Sheets

# Identification of discrepant nuclear data with machine learning

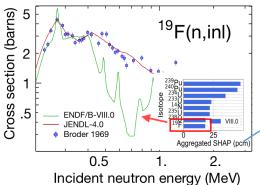
- Deficiencies in nuclear data can have significant impact on many applications, including determining USLs for criticality safety
- Previous Machine Learning project had already identified discrepant nuclear data that most contributed to bias between measured and simulated critical benchmark responses (funded by NCSP-ASC [ATDM-PEM-V&V])
- LDRD-DR project, EUCLID, objective is "to design small-scale experiments that address needs and deficiencies in nuclear data"

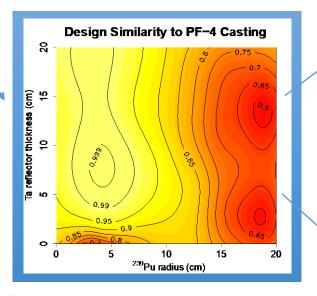


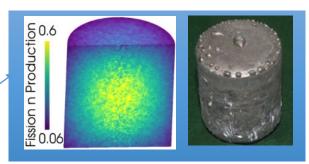


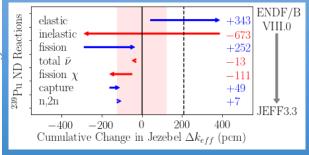
#### **Optimal experiment design**







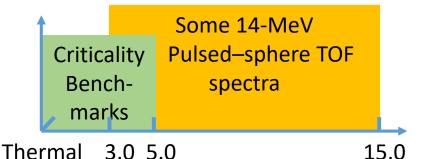




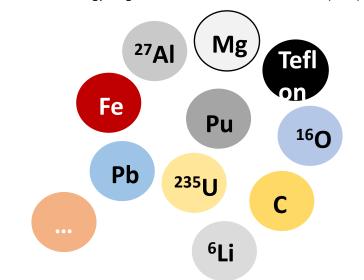


# Justification for inclusion of diverse benchmarks

- Sometimes difficult to "disentangle" which nuclear data contributes to bias in critical benchmark
  - Single integral response from critical benchmark requires ~10<sup>6</sup> differential nuclear data points to simulate
  - Difficult to consider structural/moderator/reflector material separately from fissile core
  - Sensitive to a specific region of incident neutron energies
- One approach is to apply machine learning to a diverse set of measurements
  - Integral and differential observables (e.g. k<sub>eff</sub> and TOF spectrum)
  - Composed of fissile and non-fissile materials
  - · Sensitive to nuclear data in different energy regions
- Can improve nuclear data and benefit criticality safety

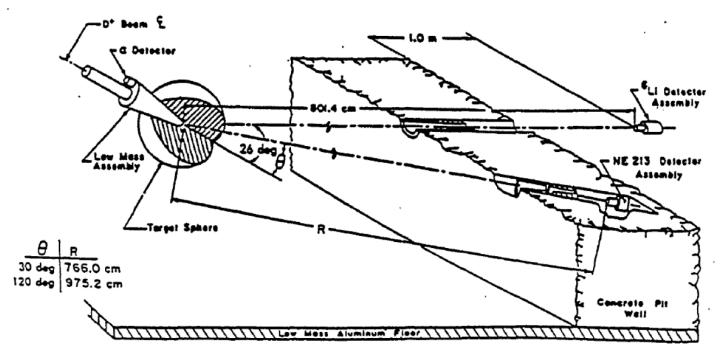


Nuclear data energy range to which simulations are sensitive (MeV)



LLNL 14-MeV pulsed spheres

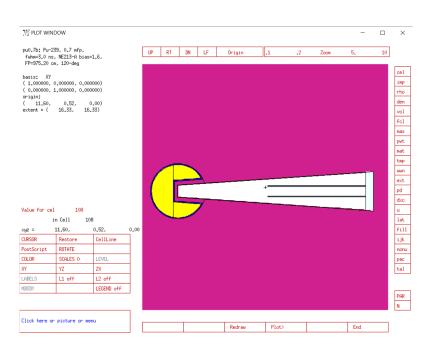
## LLNL pulsed-sphere experimental setup



1. Tanja Goričanec et al. "Analysis of the U-238 Livermore Pulsed Sphere Experiments Benchmark Evaluations," International Nuclear Data Committee Report INDC(NDS)-0742 (2017)



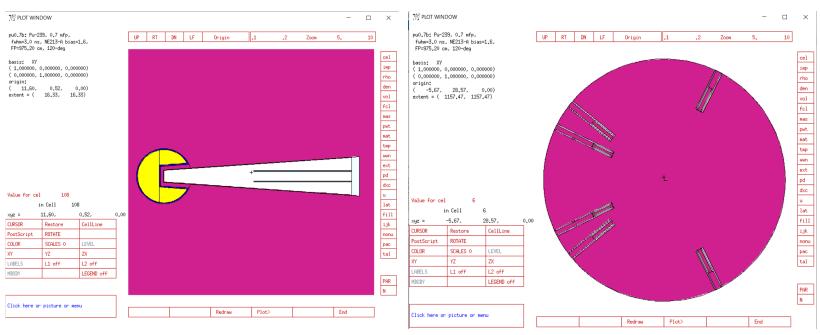
### **Pulsed-sphere MCNP model**



- 1. S.C. Frankle, "Possible Impact of Additional Collimators on the LLNL Pulsed Sphere Experiments (U)," LANL Report LA-UR-05-5877 (2005).
- 2. S.C. Frankle, "LLNL Pulsed Sphere Measurements and Detector Response Functions (U)," LANL Report LA-UR-05-5878 (2005).
- 3. S.C. Frankle, "README file for Running a LLNL Pulsed-Sphere Benchmark," LANL Report LA-UR-05-5879 (2005).



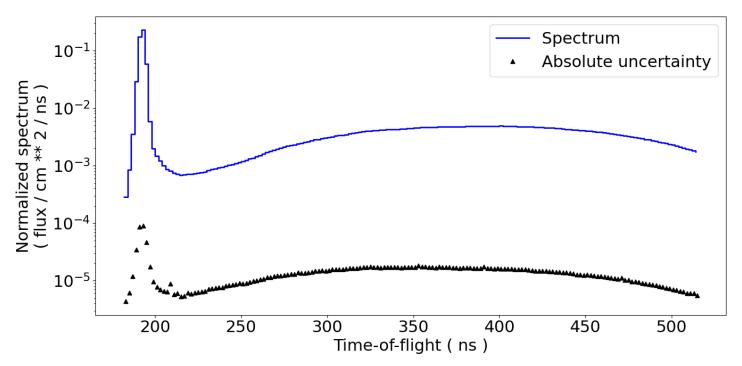
#### Pulsed-sphere MCNP model



- 1. S.C. Frankle, "Possible Impact of Additional Collimators on the LLNL Pulsed Sphere Experiments (U)," LANL Report LA-UR-05-5877 (2005).
- 2. S.C. Frankle, "LLNL Pulsed Sphere Measurements and Detector Response Functions (U)," LANL Report LA-UR-05-5878 (2005).
- 3. S.C. Frankle, "README file for Running a LLNL Pulsed-Sphere Benchmark," LANL Report LA-UR-05-5879 (2005).



#### Simulated pulsed-sphere time-of-flight spectrum for plutonium pulsed sphere



- D. Neudecker, O. Cabellos, A. R. Clark et al, "Which nuclear data can be validated with LLNL pulsed-sphere experiments?," manuscript submitted to ann. nucl. energy, Jan. 6, 2021
- 2. W. Haeck, A. R. Clark, and M. Herman, "Calculating the impact of nuclear data changes with Crater," *Trans. Am Nucl. Soc. Winter Meeting*, Online, Nov. 15-19, 2020



3/3/2021

#### Estimating sensitivities with central-difference calculations

 Sensitivity of pulsed-sphere time-of-flight spectrum to group-wise nuclear data is defined as

$$S_{R_t,\alpha_g} = \frac{\alpha_{g,0}}{R_t|_{\alpha=\alpha_{g,0}}} \frac{\partial R_t}{\partial \alpha_g} \Big|_{\alpha=\alpha_{g,0}}$$

- $R_t$  = Time-of-flight spectrum at time bin t
- $\alpha_q$  = Nuclear data parameter at group g
- Sensitivity can be numerically estimated to second-order in perturbation size with centraldifferences

$$S_{R_t,\alpha_g} = \frac{\alpha_{g,0}}{R_t|_{\alpha=\alpha_{g,0}}} \frac{R_t|_{\alpha=\alpha_{g,0}+\Delta\alpha_g} - R_t|_{\alpha=\alpha_{g,0}-\Delta\alpha_g}}{2\Delta\alpha_g} + \mathcal{O}(\Delta\alpha^2)$$



#### Sensitivity analysis procedure

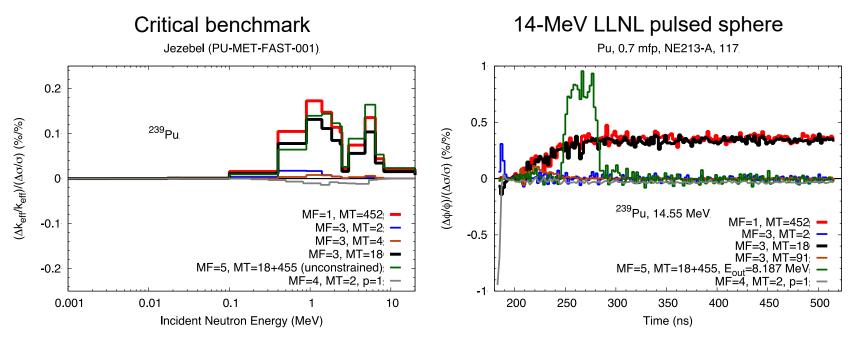
- Obtain ENDF files from nndc.bnl.gov
- Perturb nuclear data with one of two codes
  - FRENDY<sup>1,3</sup>
    - Process ENDF file into ACE format with NJOY
    - FRENDY directly perturbs ACE file
    - Operates on MF1,3
  - SANDY<sup>2,3</sup>
    - Process ENDF file into PENDF format with NJOY
    - · SANDY perturbs either ENDF or PENDF file
    - Process ENDF and PENDF files in ACE format with NJOY
    - Operates on MF3,4

- 3. Generate MCNP input decks with Faust
- 4. Perform MCNP runs on HPC machine, Snow
- 5. Post-process MCTAL files with Faust to compute sensitivities<sup>4</sup>

- 1. K. Tada et al., "Development and Verification of a New Nuclear Data Processing System FRENDY," J. Nucl. Sci. Technol., 54(7), pp. 806-817 (2017).
- 2. L. Fiorito, et al., "Nuclear data uncertainty propagation to integral responses using SANDY," Ann. Nucl. Energy, Volume 101, 2017, Pages 359-366, ISSN 0306-4549.
- 3. O. Cabellos and L. Fiorito, "Examples of Monte Carlo Techniques applied for Nuclear Data Uncertainty Propagation," EPJ Web Conf., 211 (2019) 07008
- 4. W. Haeck, A. R. Clark, and M. Herman, "Calculating the impact of nuclear data changes with Crater," Trans. Am Nucl. Soc. Winter Meeting, Online, Nov. 15-19, 2020



# Pulsed Sphere TOF spectra enable studying fission-source term observables and angular distributions differently than criticality.



1. D. Neudecker, O. Cabellos, A. R. Clark et al, "Which nuclear data can be validated with LLNL pulsed-sphere experiments?," manuscript submitted to ann. nucl. energy, Jan. 6, 2021



#### **Summary**

- Difficult to disentangle which nuclear data contribute to bias between measured and simulated experiments
- Inclusion of diverse benchmarks (e.g. critical and pulsed spheres) can inform nuclear data evaluation for a greater number of nuclides and energy regions to benefit criticality safety
  - 2-MeV LLNL pulsed sphere measurements
  - Experiment campaigns at NCERC
- Developed Python tool, Pulsed Sphere Sensitivity Analysis toolkit (PSSAtk)
- EUCLID using PSSAtk to design small-scale experiments that address needs/deficiencies in nuclear data



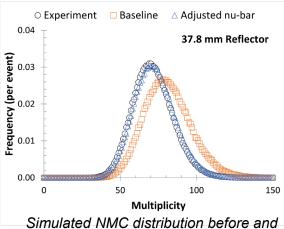
#### **Future work**

- Finish pulsed-sphere sensitivity analysis and implement parts of it into Faust
- Develop tools in Faust for covariance processing and verification
  - Check whether covariances are physically meaningful
  - Make covariances accessible for end users
- Inform adjustment of nuclear data with pulsed-sphere sensitivity and uncertainty analysis
- Demonstrate additional constraint on fission parameters improves nuclear data adjustment and benefits criticality safety

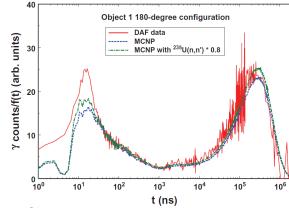


# Covariance-processing tools to benefit neutron-diagnosed subcritical experiments

- ENDF/B-VII.1 Pu-239 nu-bar reduced by ~1% to improved NMC simulations of the BeRP ball reflected by polyethylene
- ENDF/B-VII.1 U-235 inelastic scatter cross section reduced by ~20% to improve NDSE simulations of the Rocky Flats HEU shells reflected by polyethylene
- Expert knowledge identified these cross sections as high-impact to each problem
- ENDF/B-VII.1 release notes indicated that these cross sections had room in which to be adjusted
- Availability of covariance-processing tools could simplify identification and adjustment of problematic nuclear data



Simulated NMC distribution before and after Pu-239  $\overline{\nu}$  adjustment



Simulated gamma coincidence data before and after U-235 (n, n') adjustment



#### Contributions to the literature

- D. Neudecker, O. Cabellos, **A. R. Clark** et. al, "Which nuclear data can be validated with LLNL pulsed-sphere experiments?," Submitted to *Ann Nucl Energy*, Jan. 8, 2021
- J. Mattingly, **A. R. Clark**, and J. A. Favorite, "Application of Stochastic Neutron Transport Theory to Nuclear Data Evaluation using Subcritical Neutron Multiplicity Counting Experiments," accepted in Aug. 2020 for M&C2021, Raleigh, NC, Apr. 11-15, 2021
- W. Haeck, **A. R. Clark**, and M. Herman, "Calculating the impact of nuclear data changes with Crater," *Trans. Am Nucl. Soc. Winter Meeting*, Online, Nov. 15-19, 2020.
- A. R. Clark, J. Mattingly, and J. A. Favorite, "Application of neutron multiplicity counting experiments to optimal cross section adjustments," *submitted to Nucl. Sci. Eng.*, Sept. 2019
- A. R. Clark et al., "Sensitivity analysis and uncertainty quantification of the Feynman Y and Sm<sub>2</sub>," Trans. Am Nucl. Soc. Winter Meeting, Orlando, FI, Nov. 11-15, 2018
- A. R. Clark and J. Mattingly, "Data assimilation of nuclear cross sections applied to neutron multiplicity counting experiments", *Trans. Am Nucl. Soc. Annual Meeting*, Philadelphia, PA, Jun. 17-21, 2018, Invited paper



# **Supplemental content**



#### Jezebel and BeRP ball assembly comparison



Jezebel is a fast, bare, critical assembly



The BeRP ball is a fast, polyethylenereflected subcritical assembly

/3/2021

## NMC distribution vs detector response moments

• NMC distribution f(n)

• 
$$\overline{n^q} = \frac{1}{N} \sum_{n=0}^{N} n^q f(n)$$

• 
$$\mu_q = \frac{1}{N} \sum_{n=0}^{N} (n - \overline{n})^q f(n)$$

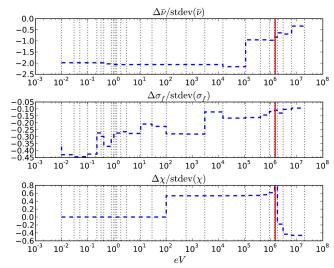
• 
$$\overline{x}_{q,r} = \frac{1}{q! N} \sum_{n=q-1}^{N} n(n-1) \dots (n-q+1) f(n)$$

- $\overline{x}_{1,r}$ ,  $\overline{x}_{2,r}$ , and  $\overline{x}_{3,r}$  are called singles, doubles, and triples
- Only moments for f(n) accumulated with large coincidence gate T are considered
- First-moment detector response  $R_1 = \frac{\overline{n}}{T}$
- Second-moment detector response  $R_2 = \frac{\mu_2 \overline{n}}{T}$



## Data assimilation applied to gross neutron counting

- Energy-dependent cross section adjustment via 3D DENOVO simulations of gross neutron counting of the BeRP ball
- Cross sections adjusted using Cacuci's data assimilation process
- Adjustment of Pu-239  $\overline{\nu}$  is between 1 and 2 standard deviations



Adjustment to the Pu-239  $\overline{\nu}$  (top),  $\sigma_f$ (middle), and  $\chi$  (bottom) in multiples of their respective standard deviations



#### Sensitivity of second-moment detector response

$$\frac{\partial R_{2}}{\partial \alpha} = \left\langle \psi_{2}^{*}, \frac{\partial Q}{\partial \alpha} - \frac{\partial L}{\partial \alpha} \psi \right\rangle + 2 \left\langle \Phi, \frac{\partial Q_{1}^{*}}{\partial \alpha} - \frac{\partial L^{*}}{\partial \alpha} \psi_{1}^{*} \right\rangle + \left\langle \frac{\partial Q_{2}^{*}}{\partial \beta}, \psi \right\rangle + \left\langle \frac{\partial Q_{2,sf}^{*}}{\partial \beta}, S \right\rangle + \left\langle Q_{2,sf}^{*}, \frac{\partial S}{\partial \alpha} \right\rangle$$

$$\beta = \left\{ \overline{\nu(\nu - 1)}, \overline{\nu(\nu - 1)}_{sf} \sigma_{f}, \chi, \chi_{sf} \right\}$$

$$L\Phi = \left\{ I_{1} \frac{\chi}{4\pi} \int d\Omega' \int dE' \overline{\nu(\nu - 1)} \Sigma_{f} \psi \right\} + \left\{ I_{1,sf} \frac{\chi_{sf}}{4\pi} \int d\Omega' \int dE' \overline{\nu(\nu - 1)}_{sf} S \right\}$$

- Φ is flux of fission neutrons that contribute to the second-moment detector response
- Second-moment detector response sensitivity calculable using standard transport solvers
- Can compute sensitivities for R<sub>3</sub> and higher-order moments in a similar way



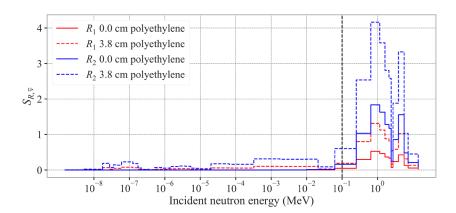
# **Definition of sensitivity vector** and total

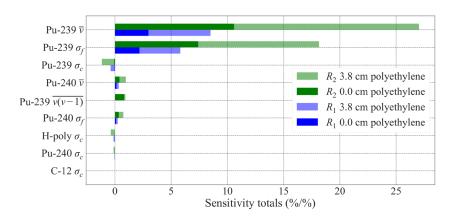
• Element of  $G \times 1$  relative sensitivity vector:

$$S_{R_q,\alpha_{g'}} = \frac{\alpha_{g'}}{R_q} \frac{\partial R_q}{\partial \alpha_{g'}}$$

Scalar relative sensitivity total:

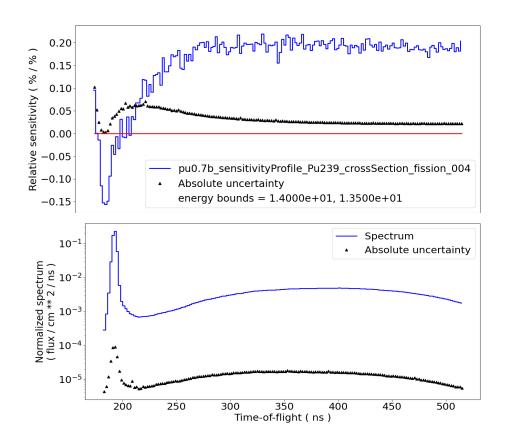
$$S_{R_q,\alpha} = \sum_{g'} S_{R_q,\alpha_{g'}}$$







## **Sensitivity to fission cross section**





#### **Sensitivity to fission cross section**

